Renormalization group study of the 1d polaron problem

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We investigate the one-dimensional polaron problem and calculate the ground state energy and the effective mass. We use a real-time renormalization group method and compare our results with first and second order perturbation theory, with Feynman's variational principle and with the method of Lee, Low and Pines.

Introduction. The polaron has often been examined since Fröhlich proposed the corresponding Hamiltonian [1,2]. It serves as a standard model for various problems involving a nonrelativistic particle moving in a scalar field, e.g. the interaction between nucleons and scalar mesons or a single electron in a solid interacting with longitudinal optical phonons. The physical picture is that the particle polarizes the environment and must drag this polarization with it, which affects its energy and effective mass. To describe the polaron not only in the weak coupling limit one has to consider it beyond perturbation theory. The most successful methods for determining the ground state energy and effective mass of the polaron are those of Lee, Low and Pines [3,4], Pekar et al. [5,6], and Feynman [7]. Since polaron effects have been observed in low-dimensional systems, the problem has also been studied in two dimensions [8–10].

In this paper we will examine the one-dimensional polaron problem. It can be realized e.g. for a Bloch-electron in a one-dimensional wire or macromolecular structure. The excitation of an electron will be strongly influenced by the interaction with optical phonons [11]. If the conduction band is partially filled, one can linearize the electronic spectrum and the model is exactly solvable by using bosonization techniques [12]. However, if the conduction band is empty, it is necessary to consider a quadratic spectrum for the electron with a bare mass m_0. This leads to the one-dimensional Fröhlich Hamiltonian with a constant coupling to the phonons. It is our purpose to examine the ground state energy and the effective mass of the electron for this problem. Thereby we will use a recently developed real-time renormalization group (RG) technique [13]. While this method actually allows nonequilibrium descriptions [14], in the present paper we have only used it to determine spectral properties. Furthermore, we will compare our results with first and second order perturbation theory, with Feynman's variational principle, and with the method of Lee, Low and Pines generalized to the one-dimensional case with finite band width. For not too large coupling constants we find a ground state energy near Feynman's method and a value for the effective mass between the result of

Feynman and the one of Lee, Low and Pines.

Model. The polaron problem is modelled by the Fröhlich Hamiltonian $H = H_0 + H_1$ with

$$H_0 = \sum_k \epsilon_k \, c_k^\dagger c_k + \sum_q \hbar \omega_q \, a_q^\dagger a_q \tag{1}$$

$$H_1 = \sum_{k,q} M_k^q \, (a_{-q}^\dagger + a_q) c_{k+q}^\dagger c_k \,. \tag{2}$$

$c_k^\dagger (c_k)$ is the creation (annihilation) operator of the electron, its energy ϵ_k is given by the electron dispersion $(\hbar k)^2/2m_0$, m_0 being the bare mass of the electron in the conduction band and $a_q^\dagger (a_q)$ creates (annihilates) a phonon with frequency ω_q. Since the interaction is dominated by the longitudinal optical branch, we presume dispersionless phonons, i.e. $\omega_q = \omega$. While the electron-phonon interaction coefficients $M_k^q \equiv M^q$ are proportional to $1/q$ in case of the bulk polaron, the one-dimensional situation involves a q-independent coefficient M [10]. We define

$$M = \left(\frac{4m_0\omega}{\hbar}\right)^{\frac{1}{4}} \frac{\sqrt{\alpha}}{\sqrt{L}} \,,$$

where L is the one-dimensional normalization volume. In analogy to the three-dimensional case α is a dimensionless coupling constant. In the following we choose units such that $\hbar = m_0 = \omega = 1$. With these assumptions the perturbation theory produces the ground state energy $E_g = -\alpha$ and the inverse effective mass $1/m = 1 - \alpha/2$.

RG method. In the RG we consider the S-matrix

$$S = T e^{-i \int dt \, H(t)}$$
$$= e^{-i \int dt \, H_0} T e^{-i \int dt \, H_1(t)_I} \,, \tag{3}$$

where $H_1(t)_I$ is the interaction part of the Hamiltonian taken in the interaction picture with respect to H_0. The idea of the RG is to leave the S-matrix invariant while successively integrating out diagrams of different time scales. The procedure is schematically shown in Fig. 1. For a given cutoff t_c in time space, we allow only for correlation functions of the phonons with a time scale $t > t_c$. At zero temperature, the latter are given by

$$\langle(a^\dagger_{-q} + a_q)(t)(a^\dagger_q + a_{-q})\rangle = e^{-i\omega t}\,. \tag{4}$$

All correlation functions with time scales shorter than t_c are accounted for by renormalized energies and coupling constants. A change of t_c to $t_c + dt_c$ is made by applying three steps [13]: (i) expanding the second exponential in (3) and introducing normal ordering for the phonon operators using Wick's theorem, (ii) integrating over the contractions with a time scale between t_c and $t_c + dt_c$ and (iii) resumming the operators in an exponential form. Consequently these operators will not be limited to zero-phonon and one-phonon operators any more. But we shall see that a good approximation is achieved for not too large coupling constants if we neglect double or higher order vertex operators. One advantage of this method is that we only need to consider the operators of the electronic system, as the phonon degrees of freedom are integrated out in each t_c-step. For the polaron problem we start with $t_c = 0$ involving the operators as in (1), (2) and end up with an effective Hamiltonian for $t_c \to \infty$. We obtain the following RG-equations

$$\frac{d\epsilon_k}{dt_c} = -i\sum_q e^{-i\Delta^q_k t_c} M^{-q}_{k+q} M^q_k \tag{5}$$

$$\frac{dM^q_k}{dt_c} = \sum_{q'}\left(M^{-q'}_{k+q+q'} M^q_{k+q'} M^{q'}_k \frac{e^{-i\Delta^{q'}_{k+q} t_c} - e^{-i\Delta^{q'}_k t_c}}{i(\Delta^{q'}_{k+q} - \Delta^{q'}_k)}\right.$$
$$\left. + M^q_k M^{-q'}_{k+q'} M^{q'}_k t_c e^{-i\Delta^{q'}_k t_c}\right)\,. \tag{6}$$

Here we introduced

$$\Delta^q_k = \epsilon_{k+q} - \epsilon_k + \omega\,.$$

The (k, q)-dependence of the interaction coefficients is generated during the RG-flow. The second term in (6) is a correction term. It is due to the fact that a time interval connected with a contraction becomes a single point in time at one RG step. In the next step this leads to the generation of new terms which were previously not present. The level broadening is also included in (5) since all energies become complex. The terms that generate the double vertex operators are of fourth order in M. Therefore the equations (5) and (6) contain the order M^4 exactly.

Feynman's method. To compare the results of the real-time RG we applied Feyman's method to the one-dimensional polaron with a finite band-width. Feynman used a variational principle in the path-integral formalism. Within his two-particle approximation one obtains for the ground state energy

$$E_g = \frac{(v - w)^2}{4v} - \alpha\frac{v}{\sqrt{\pi}}\int_0^\infty d\tau\, e^{-\tau}$$
$$\times[g(\tau)]^{-\frac{1}{2}}[\mathrm{erf}(\frac{Dg(\tau)}{v^2})^{\frac{1}{2}}] \tag{7}$$

with the band-width D, the error-function

$$\mathrm{erf(x)} = \frac{2}{\sqrt{\pi}}\int_0^x dt\, e^{-t^2}$$

and

$$g(\tau) = \left(\frac{v^2 - w^2}{v}\left(1 - e^{-v\tau}\right) + w^2\tau\right)\,.$$

v and w are chosen such that E_g is minimum. For $v = w$ the result of the perturbation theory of first order in α is reproduced. Following Feynman we treat small couplings by setting $v = (1 + \delta)w$ and $w = 1$ [15]. Considering δ small one can now expand the right-hand-side in (7) and minimize it with respect to δ. The resulting energy is

$$E_g = -\alpha\frac{2}{\pi}\arctan\sqrt{D} - \alpha^2\frac{4}{\pi^2}\left(3\arctan\sqrt{D}\right.$$
$$\left. -2\sqrt{2}\arctan\sqrt{\frac{D}{2}} - \frac{\sqrt{D}}{D+1}\right)^2\,. \tag{8}$$

Within Feynman's approximation we obtain for the effective mass:

$$m = 1 + \frac{\alpha}{\pi}\left(\arctan\sqrt{D} + \sqrt{D}\frac{D-1}{(D+1)^2}\right)$$
$$+\alpha^2\frac{4}{\pi^2}\left(3\arctan\sqrt{D} - 2\sqrt{2}\arctan\sqrt{\frac{D}{2}} - \frac{\sqrt{D}}{D+1}\right)$$
$$\times\left(-3\arctan\sqrt{D} + 3\sqrt{2}\arctan\sqrt{\frac{D}{2}}\right.$$
$$\left. + \sqrt{D}^3\frac{3D^3 + 18D^2 + 21D - 2}{(D+1)^3(D+2)^2}\right)\,. \tag{9}$$

Since (7) follows from a mininum principle Feynman's method leads to more accurate results for the energy than for the mass (for quantitative studies concerning the accuracy in three dimensions see [16]).

Our results for the energy using Feynman's approach as well as our values following from perturbation theory of second order are in good agreement with [10].

Results. The differential equations (5) and (6) are solved numerically. Regarding the oscillating terms in these equations one recognizes that given a certain discretization in q-space one obtains large errors with increasing frequency t_c. To avoid this the phase $\Delta^q_k t_c$ has been interpolated in q-space.

Unfortunately (5) and (6) do not show a convergent behaviour for the ground state energy for $t_c \to \infty$. One reason is that there are undamped modes corresponding to high excitations in the q-sums leading to increasing effects on the ground state energy. In this context another problem arises from the fact that the correlation function in (4) is not decaying. As a consequence, oscillations decay as a function of t_c but reoccur for sufficiently large t_c

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[17]. The idea of our solution is to neglect further renormalizaton effects of both Δ_k^q and M_k^q for t_c larger than a certain point t_f. By doing this we obtained a damped oscillation of the ground state energy ϵ_0 in t_c-space for $t_c > t_f$. Therefore (5) can be integrated analytically which leads to

$$
\begin{aligned}
E_g &\equiv \lim_{t_c \to \infty} \epsilon_0(t_c) \\
&= \epsilon_0(t_f) - \sum_q \frac{M_q^{-q}(t_f) M_0^q(t_f)}{\Delta_0^q(t_f)} e^{-i\Delta_0^q(t_f) t_f} .
\end{aligned} \quad (10)
$$

In Fig. 2 the solution of (10) is shown for different t_f. The problems mentioned above make it necessary to choose a finite t_f where the renormalization effects beyond perturbation theory are contained but the numerical instabilities do not yet occur. We choose $t_f = 2.5$ for all values of α. At this point only low excitations ($\Delta < 0.4$) are not integrated out yet. Since $\Delta \sim 1$ sets the scale for the first excited state, it is reasonable to assume that excited states do not have further important renormalization effects. The change of E_g between $t_f = 2$ and $t_f = 3$ is approximately 2% for $\alpha = 0.5$.

The α-dependence of E_g is shown in Fig. 3. One notices that for $\alpha < 0.7$ we obtain lower values for the ground state energy than those of Feynman's method. For larger couplings our method is no longer reliable and yields worse results (see Fig. 3) which is not surprising since we neglected double and higher order vertex operators.

We also calculated E_g for different band-widths D. As one can see in Fig. 4 for larger band-widths the deviation to the results of Feynman's method grows.

Another quantity of interest is the mass of the polaron. If one differentiates (5) twice with respect to k one obtains a differential equation for $1/m$. However, its solution oscillates with increasing amplitude. Therefore for determining the mass we calculate both the ground state energy and low excited energies using the same procedure as above. The resulting dispersion gives us a value for the mass. The accuracy for the mass is worse though. For $\alpha = 0.3$ the change of $1/m$ is approximately 6% between $t_f = 2$ and $t_f = 3$.

The results for different α are shown in Fig. 5. For small couplings ($\alpha < 0.4$), we find a value for the mass between the variational principle of Feynman and the one of Lee, Low and Pines [18]. For larger couplings the numerical solution is too unstable to make definite statements from the RG-approach. From Fig. 6 we see that our mass depends only slightly on the band-width.

In summary, we used a new renormalization group method to study the polaron problem. Although there arise some difficulties from the structure of the flow-equations, we were able to investigate the energy beyond perturbation theory. The mass was calculated as well, but its accuracy is worse than that of the energy.

The results were compared to the values following from perturbation theory, Feynman's method and the one of Lee, Low and Pines. The performance of the RG is good for couplings $\alpha \lesssim 0.5$. This restriction is due to the neglecting of double and higher order vertex operators and the undamped oscillating correlation function of the phonons.

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[15] Feynman also minimizes the energy with respect to w, but states that E_g is not sensitive to the choice of w. We found that in case of finite band-width there is no minimum with respect to w within the validity of the expansion.
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[17] We expect the numerics to be much more stable for other correlation functions, e.g. for acoustic phonons.
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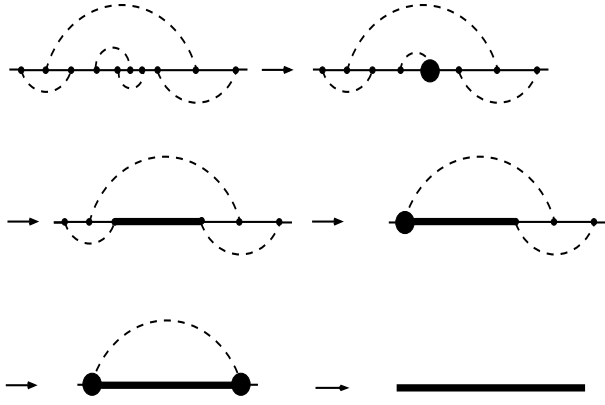
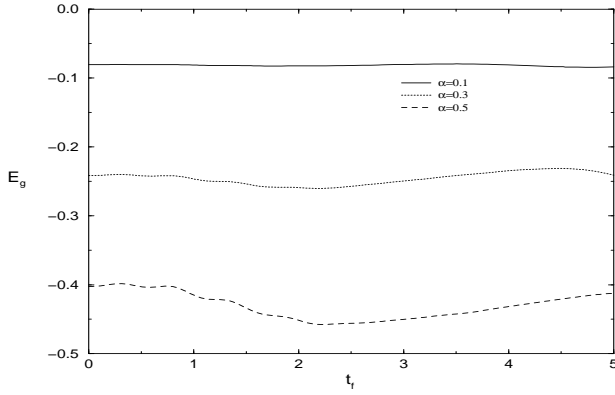FIG. 1. Scheme of the renormalization group.

FIG. 2. Ground state energy of the polaron in the renormalization group method as a function of t_f for $D = 10$. Solid line: $\alpha = 0.1$. Dotted line: $\alpha = 0.3$. Dashed line: $\alpha = 0.5$.
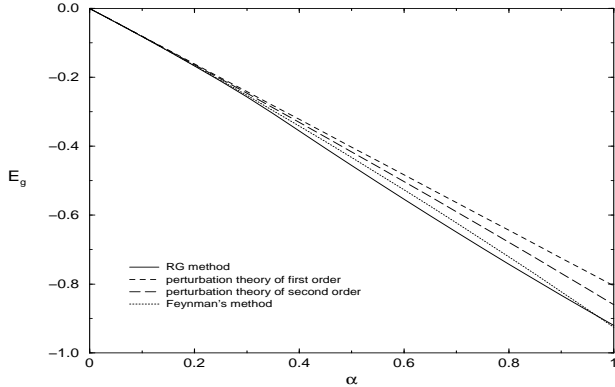

FIG. 3. Ground state energy of the polaron as a function of α for $D = 10$. Solid line: Renormalization group method described in this paper with $t_f = 2.5$. Dashed and long-dashed line: Perturbation theory of order α and α^2. Dotted line: Feynman's method.
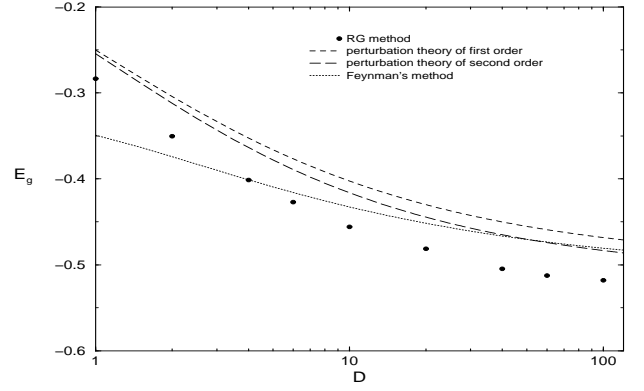

FIG. 4. Ground state energy of the polaron as a function of D for $\alpha = 0.5$. Circles: Renormalization group method described in this paper with $t_f = 2.5$. Dashed and long-dashed line: Perturbation theory of order α and α^2. Dotted line: Feynman's method.
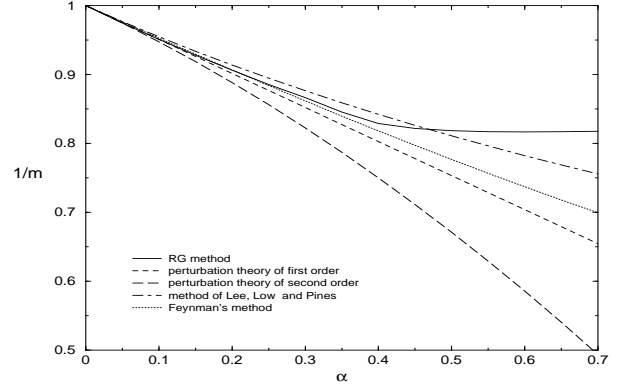

FIG. 5. Inverse mass of the polaron as a function of α for $D = 10$. Solid line: Renormalization group method described in this paper with $t_f = 2.5$. Dashed and long-dashed line: Perturbation theory of order α and α^2. Dotted line: Feynman's method. Dot-dashed line: result of Lee, Low and Pines.
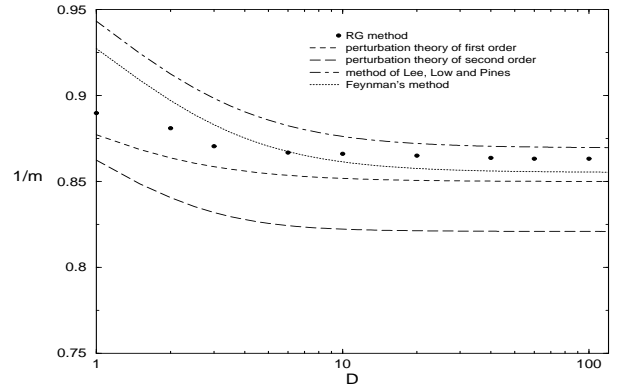

FIG. 6. Inverse mass of the polaron as a function of D for $\alpha = 0.3$. Circles: Renormalization group method described in this paper with $t_f = 2.5$. Dashed and long-dashed line: Perturbation theory of order α and α^2. Dotted line: Feynman's method. Dot-dashed line: result of Lee, Low and Pines.